

## MultiHy Update #2

November 2011

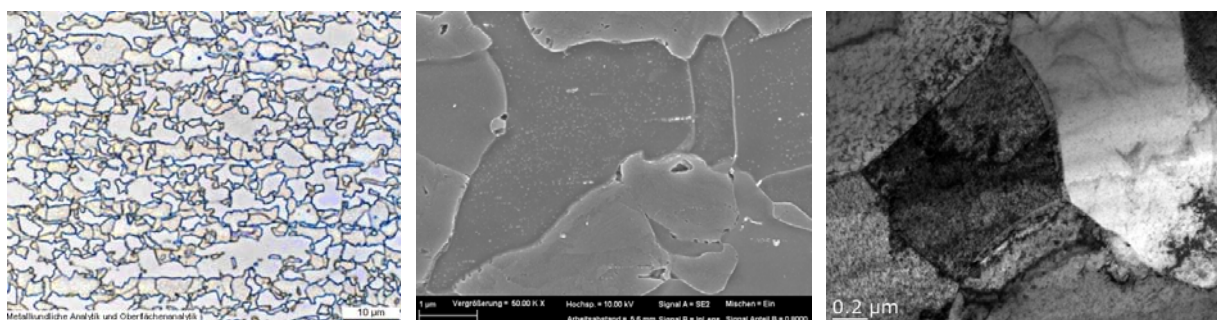
Dear Colleagues,

It is my pleasure to provide you with an update on the progress of our EU project on multiscale modelling of hydrogen embrittlement, "MultiHy", during its first six months.

Our primary objective over the last six months has been the selection and fabrication of model materials and components. These would be the focus of theoretical and experimental studies throughout the project, so it was imperative that they were delivered as early as possible in order to prevent delays in the beginning of other aspects of the project, in particular experimental work.

The process of selecting our model systems was carried out with the involvement of everyone in the consortium. In CS1 (delayed H-cracking of pulse-plated nickel), we have chosen to focus on two existing PP-Ni types, with a third type to be "tailor made" based on modelling results. In CS2 (H-assisted degradation of advanced high strength steels) we decided on steels with two basic compositions, which have been heat-treated into various grades. Nb and Ti were also added to the steels, so that we can study the effect of H trapping by carbides of these elements. In CS3 (H-assisted rolling contact fatigue of bearings) we'll focus our efforts on two common wind turbine bearing steels, which have also been heat-treated to contrasting microstructures.

To date, the majority of materials have been fabricated and have either been delivered in the form of samples or are in an advanced state of production. As a result, experimental work in WP1.4 (micromechanical testing) and WP2.1 (permeation testing) has been able to proceed without delay and is already quite advanced.



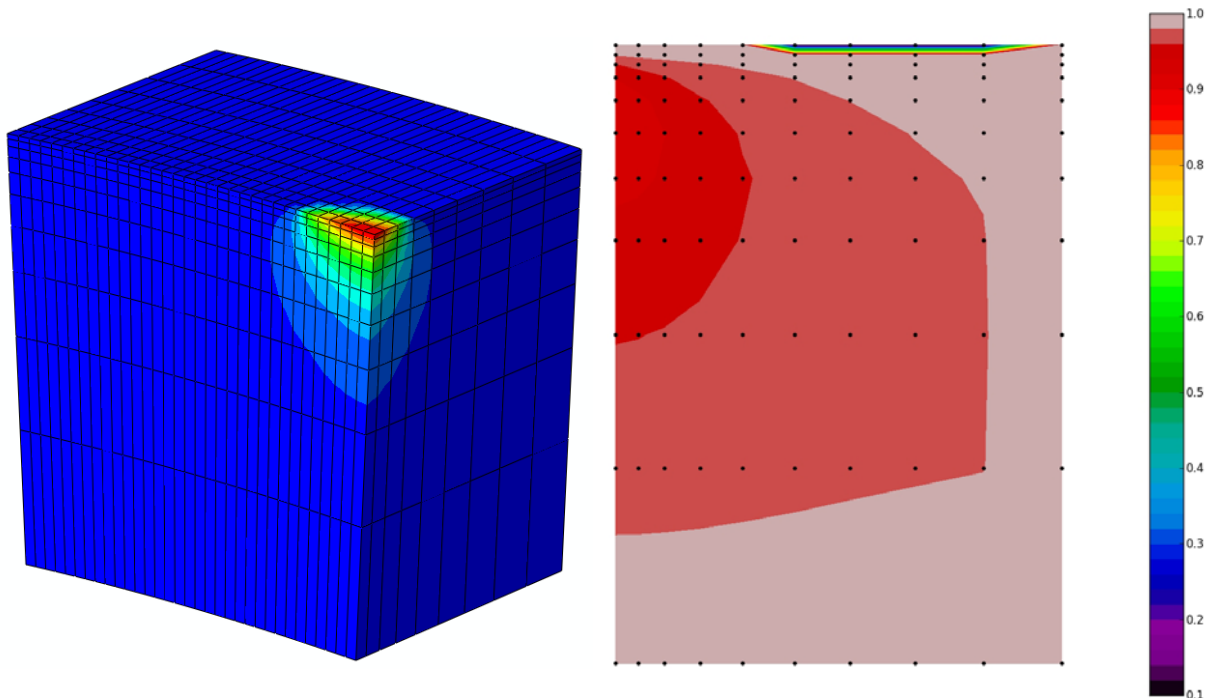
An important part of all EU projects is the dissemination and exploitation of project outcomes, which is aimed at maximising the impact of the project across all aspects of society and industry. To this end, we have established a website ([www.multihy.eu](http://www.multihy.eu)) and a promotional flyer (attached). An overview of the scope and objectives of the project was also presented at the International Conference on Steel and Hydrogen in Ghent on the 28<sup>th</sup> and 29<sup>th</sup> of September.

Efforts in WP4 (atomistic modelling) and WP5 (KMC and continuum modelling) have progress considerably during the last six months. We have developed kinetic Monte-Carlo models for H in a crystal lattice in the presence of vacancies and tight binding

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models for H and C in Fe. These will be used to study H trapping at dislocations as well as the competition between H and C for trapping by defects.

Modelling work at the continuum and component levels (i.e. finite element simulation) has not yet begun in earnest: this is not scheduled to begin until Months 6 and 12 respectively. A preliminary study of H transport and trapping under rolling contact conditions using FEM has been carried out. The results outline the importance of deformation-induced defects on the accumulation of H in critical concentrations.



In the upcoming months, we will be focusing primarily on the beginning of modelling activities at the continuum and component levels, as well as the collection of in-service data that will serve as initial and boundary conditions for the models.

As ever, we would greatly appreciate you forwarding this update (and flyer) to anyone you feel may be interested in the project.

Kind Regards

A handwritten signature in black ink, appearing to read "Nick Winzer".

Nick Winzer  
MultiHy Coordinator